

A magnetic monopole in topological insulator: exact solution and Witten effect

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The Witten effect tells that a unit magnetic monopole can bind a half elementary charge in an axion media. We present an exact solution of a magnetic monopole in a topological insulator that was proposed to be an axion media recently. It is found that a magnetic monopole can induce one zero energy state bound to it and one surface state of zero energy. The two states are quite robust, but the degeneracy can be removed by external fields. For a finite size system, the interference of two states may lift the degeneracy, and the resulting states have one half near the origin and another half around the surface, which realizes the Witten effect. However, the energy difference decays exponentially with the size of the system. The exact solution does not fully support the realization of the Witten effect in a topological insulator.

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Topological insulators are electronic materials that behave like insulators or semiconductors in the bulk, but are surrounded by a topologically protected conducting layer near the surface of the materials¹⁻³. The materials have been studied extensively. One of the predicted features in the materials is the so-called “axion electrodynamics”⁴, as an electromagnetic response to external fields. The idea of the axion was first introduced to address the strong charge-parity problem in the physics of strong interaction⁵. It becomes a possible candidate for the dark matter in the universe, and however, has not been yet confirmed experimentally so far. Historically, it was known that an additional term $\theta \frac{e^2}{2\pi h} \mathbf{B} \cdot \mathbf{E}$ can be introduced into the Maxwell Lagrangian for electric and magnetic fields, which is time reversal invariant when $\theta = \pi$. The additional term revises both the Gauss’ law and Ampere’s law in the Maxwell’s equations by adding extra terms⁶,

$$\nabla \cdot \mathbf{D} = \rho_e - \frac{\alpha}{\pi \mu_0 c} \nabla \theta \cdot \mathbf{B}, \quad (1)$$

$$\nabla \times \mathbf{H} = \partial_t \mathbf{D} + \mathbf{j} + \frac{\alpha}{\pi \mu_0 c} (\nabla \theta \times \mathbf{E} + \partial_t \theta \mathbf{B}) \quad (2)$$

where $\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}$ and $\mathbf{H} = \frac{1}{\mu_0} \mathbf{B} - \mathbf{M}$. The fine structure constant $\alpha = \frac{e^2}{2\epsilon_0 h c}$. One of the fundamental properties in the revised Maxwell’s or axion equations is the Witten effect, which states that a magnetic monopole of unit strength $e_M = \phi_0 = \frac{h}{e}$ in an axion media must bind an electric charge, $-(n + \frac{\theta}{2\pi})e$, where $e(>0)$ the elementary charge and n is an integer. Consider a point-like magnetic monopole situated at the origin. The magnetic field is given by $\nabla \cdot \mathbf{B} = \phi_0 \delta(\mathbf{r})$. We suppose that $\theta = 0$ initially and then increases adiabatically to $\theta = \pi$. θ is uniform in the space and there is no current in the media. It follows from the axion equations that

$$\delta \rho_e = \rho_e(\theta = \pi) - \rho_e(\theta = 0) = -\frac{\alpha}{\mu_0 c} \nabla \cdot \mathbf{B} = -\frac{e}{2} \delta(\mathbf{r}). \quad (3)$$

As a magnetic monopole cannot induce a half elementary charge in a conventional media of $\theta = 0$, the charge

bound to the monopole should be $-e/2$ except for an integer for a time reversal invariant topological insulator of $\theta = \pi$ ⁷. Charge fractionalization in condensed matters was extensively discussed in 1980s^{8,9}. The quasi-particles in the fractional quantum Hall effect carry fractional charge^{10,11}. Whether or not a half elementary charge bound by a magnetic monopole could exist in a topological insulator becomes a subtle issue to test the validity of the axion theory for topological insulators. Rosenberg and Franz studied the Witten effect in a crystalline topological insulator numerically¹², and intended to use it as a criterion to justify whether the system is topologically trivial or non-trivial¹³.

In this paper, we present an exact solution of a magnetic monopole located in the center of a sphere of a topological insulator, which is described by a modified Dirac-like equation. It is found that there exist two solutions of zero energy: one is located in the vicinity of the magnetic monopole and the other around the surface, which is characteristic of non-trivial topological insulator. At half filling, only one electron occupies the two degenerate states due to the particle-hole symmetry in the system. The double degeneracy of the zero energy states does not favor or disfavor the Witten effect because the bound charge near the monopole can be from zero to $-e$, although it does not exclude a half elementary charge as the Witten effect requires. The degeneracy of the two states can be removed due to the finite size effect for a small sphere. In the case the occupied state have one half in the vicinity of the monopole, and another half is distributed around the surface, in which the Witten effect can be realized. In general, the external fields such as the Zeeman field and electric potential can remove the degeneracy of the two states, but could not mix them to realize the Witten effect.

The model Hamiltonian for a magnetic monopole in the modified Dirac equation is given by¹⁴

$$H = \begin{pmatrix} mv^2 - B\Pi^2 & v\sigma \cdot \Pi \\ v\sigma \cdot \Pi & -mv^2 + B\Pi^2 \end{pmatrix} \quad (4)$$

where $2mv^2$ is the energy gap between the conduction

band and valence band, v is the effective velocity and B is a parameter of dimension of inverse mass. $\sigma_{x,y,z}$ are the Pauli matrices. The canonical momentum operator $\Pi = -i\hbar\nabla + e\mathbf{A}$ and $\nabla \times \mathbf{A} = \frac{2q}{4\pi}\phi_0\mathbf{r}/r^3$. q is half of an integer due to the quantization of magnetic charge and $q = \frac{1}{2}$ for a unit monopole¹⁶. It is known that the vector potential \mathbf{A} cannot be written as a single expression in the whole space, and has to be defined as two functions in two overlapping regions to keep singular¹⁷. In the absence of the magnetic monopole, the topological properties of this equation have been studied extensively. It is topologically non-trivial for $mB > 0$ and trivial for $mB < 0$. A topological quantum phase transition occurs at $mB = 0$ ^{14,15}. In the presence of the magnetic monopole, the orbital angular momentum is modified to $\mathbf{L} = \mathbf{r} \times \Pi - q\hbar\frac{\mathbf{r}}{r}$, which satisfies the algebra $[\mathbf{L}_\alpha, \mathbf{L}_\beta] = i\hbar\epsilon_{\alpha\beta\gamma}\mathbf{L}_\gamma$. The eigenfunctions of \mathbf{L}^2 and \mathbf{L}_z are denoted by Y_{q,l,l_z} with the eigenvalues $l(l+1)\hbar^2$ and $l_z\hbar$. Since the two terms in \mathbf{L} are orthogonal to each other, $\mathbf{L}^2 = |\mathbf{r} \times \Pi|^2 + q^2\hbar^2$ and $l(l+1) \geq q^2$ ¹⁸. The total angular momentum is defined as $\mathbf{J} = \mathbf{L} + \frac{\hbar}{2}\sigma$. The total angular momentum \mathbf{J}^2 and its z-component \mathbf{J}_z commute with the Hamiltonian, and are good quantum numbers. Thus we can diagonalize simultaneously H , \mathbf{J}^2 and \mathbf{J}_z . According to the definition, \mathbf{J} is the sum of two angular momenta, \mathbf{L} and σ . Thus the eigenvalues of \mathbf{J}^2 can be $j = l + \frac{1}{2}$ and $j = l - \frac{1}{2}$, respectively, and the corresponding eigenstates are the linear combination of Y_{q,l,l_z} and the eigenvector for σ_z . For a minimal $l(=|q|)$ and $j = |q| - \frac{1}{2}$, the eigenstates are

$$\eta_{j,j_z} = \begin{pmatrix} -\sqrt{\frac{|q|-m+\frac{1}{2}}{2|q|+1}}Y_{q,|q|,j_z-\frac{1}{2}} \\ \sqrt{\frac{|q|+m+\frac{1}{2}}{2|q|+1}}Y_{q,|q|,j_z+\frac{1}{2}} \end{pmatrix}. \quad (5)$$

Due to the particle-hole symmetry in the model Hamiltonian, the eigenvalues of $\pm E$ appear in pairs. For a half-filled system, we are interested in the energy levels near the Fermi surface at $E = 0$ if it exists. Thus we focus on the case of $l = |q|$ and $j = |q| - \frac{1}{2}$ while other cases of j and l may have the eigenstates below or above than the Fermi level. To solve the problem, using the relations¹⁸, $(\sigma \cdot \mathbf{r})\eta_{j,j_z} = r\text{sgn}(q)\eta_{j,j_z}$ and $\sigma \cdot \Pi f(r)\eta_{j,j_z} = -i\text{sgn}(q)(\partial_r + r^{-1})f(r)\eta_{j,j_z}$, where $f(r)$ are arbitrary function of r , we construct a simultaneous eigenstate for H , \mathbf{J}^2 and \mathbf{J}_z :

$$\psi_{j,m} = \begin{pmatrix} f(r)\eta_{j,j_z} \\ g(r)\eta_{j,j_z} \end{pmatrix} \equiv \begin{pmatrix} f(r) \\ g(r) \end{pmatrix} \otimes \eta_{j,j_z}. \quad (6)$$

The equation for the radial part of the wave function is reduced into

$$\left\{ \left[1 + \text{sgn}(mB) \left(\partial_\rho^2 - \frac{|q|}{\rho^2} \right) \right] \sigma_z - i\zeta \partial_\rho \sigma_x - \lambda \right\} \begin{pmatrix} \rho f \\ \rho g \end{pmatrix} = 0 \quad (7)$$

Here $\rho = kr$ ($k^2 = |mv^2/B\hbar^2|$), $\zeta = \text{sgn}(qmv)/\sqrt{|mB|}$ and $\lambda = E/mv^2$.

We first consider a large radius limit of the sphere, $kR \gg 1$. In this case it is reduced to a one-dimensional

modified Dirac equation by ignoring the term of $\frac{q}{\rho^2}$ at the end of $r = R$: the sign of mB determines whether there exists a solution of zero energy solution near $r = R$ ¹⁴. For $\lambda = 0$, there is a general solution

$$\psi_{j,m}^s = \chi_s \otimes \eta_{j,j_z} f_s(\rho) \quad (8)$$

with $\sigma_y \chi_s = s \chi_s$ ($\chi_s^T = \frac{1}{\sqrt{2}}(1, is)$ and ($s = \pm 1$)). For $\zeta^2 \neq 4$

$$f_s(\rho) = C_1 e^{-s\zeta\rho/2} \frac{1}{\sqrt{\rho}} J_\alpha(\beta\rho) + C_2 e^{-s\zeta\rho/2} \frac{1}{\sqrt{\rho}} K_\alpha(\beta\rho). \quad (9)$$

where $J_\alpha(x)$ and $K_\alpha(x)$ ($\alpha = \sqrt{|q| + \frac{1}{4}}$ and $\beta = \sqrt{1 - \zeta^2/4}$) are the first and second Bessel functions, and C_i ($i = 1, 2, 3, 4$) is the normalization constant. For $\zeta^2 > 4$ or an imaginary β the solution is still valid. We can also use the modified Bessel functions to replace the Bessel functions. Consider the boundary condition at $\rho = 0$ and $\rho = kR = \rho_R$. We have two solutions of zero energy. For $s = 1$ by taking $\zeta > 0$ without losing generality, one has a solution which is convergent at $\rho = 0$, but decays exponentially with a larger ρ

$$f_+(\rho) = C_1 e^{-|\zeta|\rho/2} \frac{1}{\sqrt{\rho}} J_\alpha(\beta\rho). \quad (10)$$

Thus the wave function denoted by $\psi_{j,m}^+(\rho) = \chi_+ \otimes \eta_m f_+(\rho)$ is mainly located near the origin or the magnetic monopole. On the other hand, both $J_\alpha(\beta\rho)$ and $K_\alpha(\beta\rho)$ become divergent for a large ρ , but convergent for a small ρ . For $s = -1$ one has the other solution which vanishes at $\rho_R = kR$

$$f_-(\rho) = C_1 \frac{\sqrt{\rho_R} e^{|\zeta|\rho/2}}{\sqrt{\rho} e^{|\zeta|\rho_R/2}} \left(\frac{J_\alpha(\beta\rho)}{J_\alpha(\beta\rho_R)} - \frac{K_\alpha(\beta\rho)}{K_\alpha(\beta\rho_R)} \right). \quad (11)$$

This solution denoted by $\psi_{j,m}^-(\rho) = \chi_- \otimes \eta_m f_-(\rho)$ is distributed near the surface of $r = R$ and decays exponentially in $\rho_R - \rho$ or $R - r$. This is a surface state of zero energy, and is one of the characteristics of topological insulators. For $\zeta^2 = 4$ and $\beta = 0$, we also have two solutions of zero energy: one is near the origin,

$$f_+(\rho) = C_3 e^{-|\zeta|\rho/2} \rho^{\alpha-1/2} \quad (12)$$

with $s = 1$ and the other is around the surface,

$$f_-(\rho) = C_4 \frac{e^{|\zeta|\rho/2}}{e^{|\zeta|\rho_R/2}} \left(\left(\frac{\rho}{\rho_R} \right)^{\alpha-\frac{1}{2}} - \left(\frac{\rho_R}{\rho} \right)^{\alpha+\frac{1}{2}} \right) \quad (13)$$

with $s = -1$.

Except for the two solutions of zero energy, there also exist other states even for $l = |q|$ and $j = |q| - \frac{1}{2}$. We solve Eq. (7) numerically, and present the results in Fig. 1. We note that the solutions of zero energy appear only for the case of $mB > 0$. There is no solution of zero energy

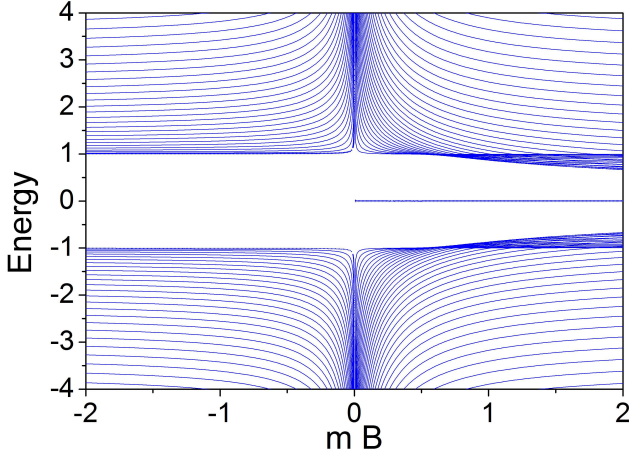


FIG. 1: Energy spectrum of the bound states of $l = |q| = \frac{1}{2}$ and $j = l - \frac{1}{2}$ as a function of the dimensionless parameter mB . The energy unit is $|m|v^2$. In general, the states of the zero energy is $4|q|$ -fold degeneracy.

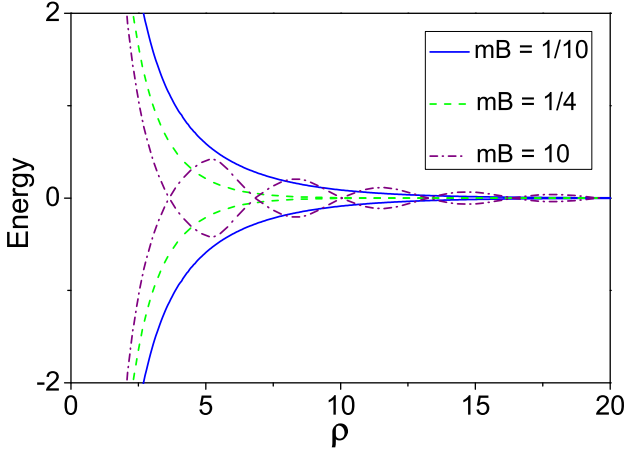


FIG. 2: The energy splitting of the two bound states as a function of the spherical radius $\rho_R = kR$. The energy unit is $|m|v^2$ and $k^2 = |mv^2/B\hbar^2|$.

for $mB < 0$ as the system is topologically trivial. We find that all other states are not the surface states, but the bound states like those with different total quantum numbers in a hydrogen atom. As the results are independent of j_z , all these states are $2(2j+1) = 4|q|$ -fold degenerate. For $q = \pm\frac{1}{2}$, the states are singlet with total angular momentum $j = 0$. Due to the topology of the band structures in topological insulator the existence of the surface state is robust against the continuous deformation of the surface shape, impurities or interaction while the zero energy state around the magnetic monopole is located very close to the origin, although the energy eigenvalues may shift away from the zero energy.

In the present case of half filling, the Fermi level is located at $E = 0$ due to the particle-hole symmetry in Eq.(4), below which all states or levels are fully filled. Al-

though we do not obtain general solutions of other states of different j and j_z , some of which are the surface states between the energy gap, the double degenerated states at $E = 0$ are closely related to possible realization of the Witten effect. For $q = \frac{1}{2}$, there is only one electron to occupy these two well-separated states. When $mB < 0$, there is no solutions of zero energy near the center and around the surface. Although it is possible that the magnetic monopole can bind a lot of electrons with the energy below zero, the electron charges accumulated around it must be an integer multiple of the elementary charge $-e$. This is consistent with the fact that the system is topologically trivial with $\theta = 0$. When $mB > 0$, the system is topologically non-trivial. the appearance of the surface state of $E = 0$ is one of the characteristics. If the topological insulator is really an axion media, θ should be π . Thus the sign change of mB should accompany the change of θ from 0 to π . Therefore if a topological insulator is really an axion media, a half elementary charge must be bound to the magnetic monopole as the Witten effect requires. Since the doubly degenerate states are well separated in space, our exact solutions do not favor or disfavor the picture of the Witten effect as the the charge bound to the monopole can be from 0 to $-e$.

Now we come to consider a sphere of a finite radius R . Denote the state near the origin by $\psi_{j,m}^+$ and the surface state by $\psi_{j,m}^-$. If the radius is large enough such that the two wavefunctions have no overlap in space, $\psi_{j,m}^+$ and $\psi_{j,m}^-$ are two exact solutions of zero energy. However, when the radius R is finite and the two wavefunctions overlap in space, the two wavefunctions interference with each other, and the degeneracy can be lifted, which is dubbed the finite size effect¹⁹. As an degenerated perturbation approach, we still use the two functions as the basis. As χ_s are the eigenstates of σ_y , we have the relations $\chi_s^\dagger \sigma_z \chi_s = \chi_s^\dagger \sigma_x \chi_s = 0$. Therefore the expectation values $\langle \psi_{j,m}^\pm | H | \psi_{j,m}^\pm \rangle \equiv 0$. However, $\chi_s^\dagger \sigma_z \chi_{-s} = 2$ and $\chi_s^\dagger \sigma_x \chi_{-s} = -2is$, then $\Delta = \langle \psi_{j,m}^+ | H | \psi_{j,m}^- \rangle \neq 0$. As a consequence of the first-order degenerate perturbation, the energy eigenvalues become $\pm|\Delta|$ and the two states become

$$\psi_\pm = \frac{1}{\sqrt{2}} \left(\psi_{j,m}^+ \pm \frac{\Delta}{|\Delta|} \psi_{j,m}^- \right). \quad (14)$$

The values of the $\pm|\Delta|$ are evaluated numerically and plotted in Fig.2. There are two different cases. For $\zeta^2 \leq 4$, the gap increases monotonically with decreasing R while for $\zeta^2 > 4$ the gap oscillates, but the amplitude increases with decreasing R . The states ψ_\pm are separated into two halves as $\psi_{j,m}^+$ and $\psi_{j,m}^-$ are orthogonal and well separated in space. The weights of these two parts are exactly equal to $1/2$. When the state with lower energy is occupied, the electron will be split into two parts: one half is near the origin and the other is around the surface as shown in Fig. 3. Thus the fractional charge is indeed realized in this case. To estimate the size of the wave package in real materials, we adopt

the fitted parameters from ARPES data for Bi_2Se_3 ²⁰: $mv^2 = 0.126\text{eV}$, $B\hbar^2 = 21.8\text{eV}\text{\AA}^2$, and $\hbar v = 2.94\text{eV}\text{\AA}$. As the wave function decays exponentially combining a power law decay from the origin, $\exp[-r/\xi]$ or from the surface, $\exp[-(R-r)/\xi]$, the characteristic length is $\xi \simeq 15\text{\AA}$. The finite size effect becomes obvious when R is comparable with several $2\xi \simeq 30\text{\AA}$, which is consistent with the fact that gap opening in the Bi_2Se_3 thin film with thickness several quintuple layers^{15,20}. Therefore the characteristic length for a finite size effect is quite small. Rosenberg and Franz claimed that a half electron charge is really bound to a magnetic monopole in a crystalline topological insulator¹². In their numerical calculation, the lattice size is of 20^3 for a cubic lattice. The finite size effect is obviously seen from the distribution of excess charge: the size for the bound state around the monopole is about 4-5 lattice spaces and that for the surface state is about 6-7 lattice spaces. Thus what observed in their calculation is actually a finite size effect.

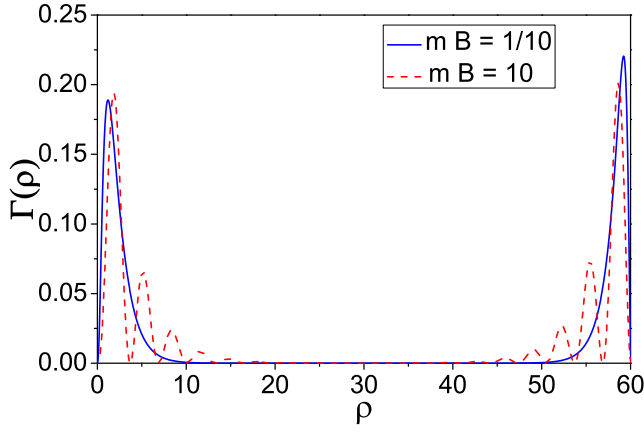


FIG. 3: The radial probability density $\Gamma(\rho) = \rho^2 (|f|^2 + |g|^2)$ with a radius $\rho_R = kR = 60$. The energy unit is $|m|v^2$ and $k^2 = |mv^2/B\hbar^2|$.

Another question is whether charge fractionalization can be realized by the Zeeman field in the topological insulator or due to the proximity effect of a ferromagnetic layer covering around the surface. Consider a radial field $\mathbf{B} = B_r \frac{\mathbf{r}}{r}$. The Zeeman energy term is

$$\delta H = \mu_{eff} B_r \begin{pmatrix} \sigma_r & 0 \\ 0 & \sigma_r \end{pmatrix}, \quad (15)$$

which breaks the time reversal symmetry. The energy shifts of the two states of zero energy are $\Delta E_{\pm} = 2\text{sgn}(q)\mu_{eff} \int_0^{\rho_R} d\rho B_r |f_{\pm}(\rho)|^2$. The degeneracy will be removed as the two integrals are usually not equal. For example, if the field appears only near the surface due to the proximity effect of a ferromagnetic layer, it is obvious that $\Delta E_+ = 0$ and $\Delta E_- \neq 0$. However, as the off-diagonal integral is zero, $\langle \psi_{j,m}^+ | \delta H | \psi_{j,m}^- \rangle = 0$, the two states will never be mixed as those due to the finite size effect. Essentially the two states are still located near the origin and the surface separately even in the presence of the Zeeman field. Also a weak and radial potential $V(r)$ can also remove the degeneracy of the two bound states, although the two states are still robust.

In short the exact solutions of a magnetic monopole with strength ϕ_0 in a topological insulator do not fully support the Witten effect, a key feature of an axion media. This raises a question whether a topological insulator is really an axion media as predicted by topological field theory or not. The finite size effect may produce the Witten effect, which suggests that topological insulators are very close to an axion media. The solutions also demonstrate that a magnetic monopole can induce spinless bound state, which is a rare example of the spin-charge separation in three dimensions.

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